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=> d his

     (FILE 'HOME' ENTERED AT 11:16:37 ON 05 MAY 2008)

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L5           4 S L4  SUB=L3 FUL
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L7           1 S L5 AND CAPLUS/LC

     FILE 'CAPLUS' ENTERED AT 11:23:41 ON 05 MAY 2008
L8          10 S L3
L9           1 S L5
L10         10 S L8 OR L9

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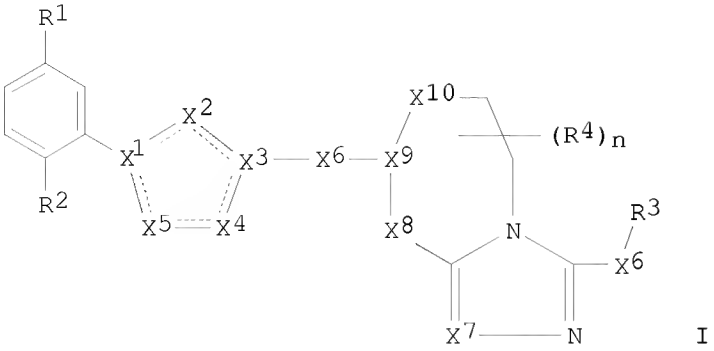
L10 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:962262 CAPLUS
DOCUMENT NUMBER: 143:248419
TITLE: Preparation of heterocyclic-fused 1,3-diazenes and analogs as metabotropic glutamate receptor antagonists
INVENTOR(S): Johansson, Martin; Wensbo, David; Minidis, Alexander; Staaf, Karin; Kers, Annika; Edwards, Louise; Isaac, Methvin; Stefanac, Tomislav; Slassi, Abdelmalik; McLeod, Donald
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; NPS Pharmaceuticals, Inc.
SOURCE: PCT Int. Appl., 69 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2005080397	A2	20050901	WO 2005-US5218		20050217
WO 2005080397	A3	20051222			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, SM					
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
AU 2005214380	A1	20050901	AU 2005-214380		20050217
CA 2556320	A1	20050901	CA 2005-2556320		20050217
EP 1716152	A2	20061102	EP 2005-713794		20050217
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, BA, HR, IS, YU					
CN 1934112	A	20070321	CN 2005-80008454		20050217
BR 2005007495	A	20070710	BR 2005-7495		20050217
JP 2007523183	T	20070816	JP 2006-554237		20050217
US 20060009443	A1	20060112	US 2005-60560		20050218
IN 2006DN04525	A	20070824	IN 2006-DN4525		20060804
NO 2006003562	A	20061106	NO 2006-3562		20060807
MX 2006PA09018	A	20061207	MX 2006-PA9018		20060807
US 20070185095	A1	20070809	US 2007-588699		20070309
PRIORITY APPLN. INFO.:			US 2004-545580P	P	20040219
			US 2004-545288P	P	20040218
			WO 2005-US5218	W	20050217

OTHER SOURCE(S): MARPAT 143:248419
GI



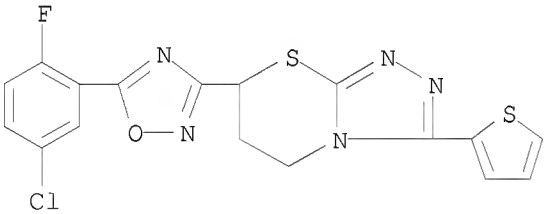
I

AB Title compds. I [X1-5 = C, CR5, N, O, S wherein at least one is not N; X6 = bond, divalent carbon; X7 = CR5, N; X8 = bond, divalent carbon, etc.; X9 = CR5, N; X10 = bond, divalent carbon, etc.; R1 = OH, halo, NO2, etc.; R2 = H, OH, halo, etc.; R3 = 5-6 membered ring; R4 = OH, halo, NO2, etc.; R5 = H, alkyl, cycloalkyl, aryl; n = 0-4 with some provisions] are prepared For instance, 7-[5-(5-Chloro-2-fluorophenyl)-1,2,4-oxadiazol-3-yl]-3-(2-thienyl)-6,7-dihydro-5H-[1,2,4]triazolo[3,4-b][1,3]thiazine is prepared by cyclization of 2-[3-[[[5-(5-chloro-2-fluorophenyl)-1,2,4-oxadiazol-3-yl]methyl]thio]-5-(2-thienyl)-4H-1,2,4-triazol-4-yl]ethyl methanesulfonate (DMF, NaH). Compds. of the invention have IC50 < 10 μM for the mGluR5 receptor. I are useful for the treatment of gastrointestinal disorders.

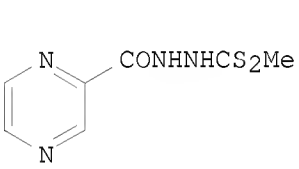
IT 863307-58-8P, 7-[5-(5-Chloro-2-fluorophenyl)-1,2,4-oxadiazol-3-yl]-3-(2-thienyl)-6,7-dihydro-5H-[1,2,4]triazolo[3,4-b][1,3]thiazine
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclic-fused 1,3-diazenes and analogs as metabotropic glutamate receptor antagonists)

RN 863307-58-8 CAPLUS

CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazine, 7-[5-(5-chloro-2-fluorophenyl)-1,2,4-oxadiazol-3-yl]-6,7-dihydro-3-(2-thienyl)- (CA INDEX NAME)



L10 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:25972 CAPLUS
DOCUMENT NUMBER: 142:447183
TITLE: Studies on pyrazine derivatives. XL. Synthesis, reactivity, and tuberculostatic activity of 4-(hydroxyalkyl)-5-pyrazinyl-4H-[1,2,4]triazole-3-thiones
AUTHOR(S): Foks, Henryk; Janowiec, Mieczyslaw; Zwolska, Zofia; Augustynowicz-Kopec, Ewa
CORPORATE SOURCE: Department of Organic Chemistry, Medical University of Gdansk, Pol.
SOURCE: Phosphorus, Sulfur and Silicon and the Related Elements (2004), 179(12), 2519-2526
CODEN: PSSLEC; ISSN: 1042-6507
PUBLISHER: Taylor & Francis, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:447183
GI



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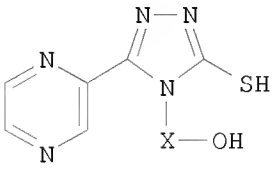

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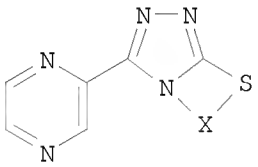


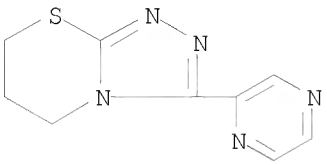
III

AB In the reactions of pyrazinoyldithiocarbazoic acid monoester (I) with amino alcs., 4-(hydroxyalkyl)-1,2,4-triazole-3-thiones [II; X = (CH2)2, (CH2)3, CH2CHMeCH2] were obtained. Their susceptibility to alkylation, as well as their heterocyclization to III (same X), were examined Some of the compds. obtained were tested for their tuberculostatic activity.

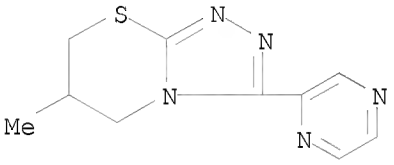
IT 717847-90-0P 851052-20-5P 851052-21-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, alkylation, and heterocyclization of (hydroxyalkyl)pyrazinyltriazolethiones)

RN 717847-90-0 CAPLUS

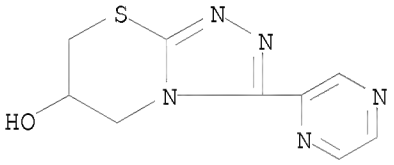
CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazine, 6,7-dihydro-3-pyrazinyl- (9CI) (CA INDEX NAME)



RN 851052-20-5 CAPLUS
CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazine, 6,7-dihydro-6-methyl-3-(2-pyrazinyl)- (CA INDEX NAME)



RN 851052-21-6 CAPLUS
CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazin-6-ol, 6,7-dihydro-3-(2-pyrazinyl)- (CA INDEX NAME)



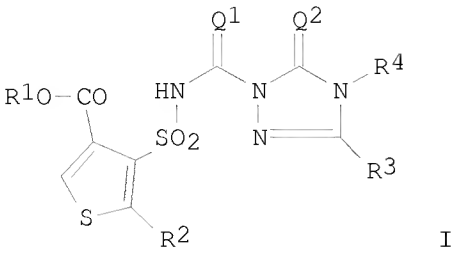
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:356160 CAPLUS
DOCUMENT NUMBER: 138:333193
TITLE: Preparation of thien-3-yl-sulfonylamino(thio)carbonyltriazolin(thi)one derivatives as herbicides
INVENTOR(S): Gesing, Ernst-Rudolf; Drewes, Mark Wilhelm; Dahmen, Peter; Feucht, Dieter; Pontzen, Rolf
PATENT ASSIGNEE(S): Bayer CropScience AG, Germany
SOURCE: PCT Int. Appl., 104 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003037086	A1	20030508	WO 2002-EP11743	20021021
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10154074	A1	20030515	DE 2001-10154074	20011102
IN 2002MU00904	A	20050121	IN 2002-MU904	20021017
CA 2465079	A1	20030508	CA 2002-2465079	20021021
AU 2002340585	A1	20030512	AU 2002-340585	20021021
EP 1443822	A1	20040811	EP 2002-774735	20021021
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
BR 2002014097	A	20040928	BR 2002-14097	20021021
CN 1578625	A	20050209	CN 2002-821549	20021021
JP 2005507403	T	20050317	JP 2003-539443	20021021
RU 2316555	C2	20080210	RU 2004-116822	20021021
MX 2004PA04020	A	20040723	MX 2004-PA4020	20040428
US 20050014809	A1	20050120	US 2004-493894	20040816

PRIORITY APPLN. INFO.: DE 2001-10154074 A 20011102
WO 2002-EP11743 W 20021021

OTHER SOURCE(S): MARPAT 138:333193
GI



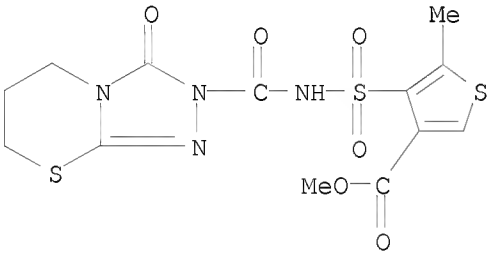
I

AB The thien-3-yl-sulfonylamino(thio)carbonyl-triazolin(thi)ones I [Q1, Q2 = O or S; R1 = (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, aryl, etc.; R2 = H, CN, NO2, halo (un)substituted alkyl, alkoxy, etc.; R3 = H, OH, SH, NH2, CN, halo, (un)substituted alkyl, alkenyl, alkynyl, etc.; R4 = H, OH, NH2, CN, alkylidenamino, (un)substituted alkyl, alkenyl, alkynyl, etc.] are prepared as herbicides. A number of known compds. are excluded.

IT 517883-79-3P 517885-09-5P 517885-48-2P
RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation as herbicide)

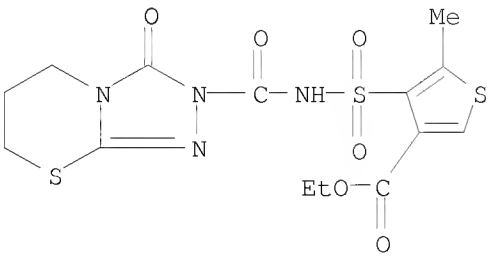
RN 517883-79-3 CAPLUS

CN 3-Thiophenecarboxylic acid, 4-[[[(6,7-dihydro-3-oxo-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-2(3H)-yl)carbonyl]amino]sulfonyl]-5-methyl-, methyl ester (CA INDEX NAME)

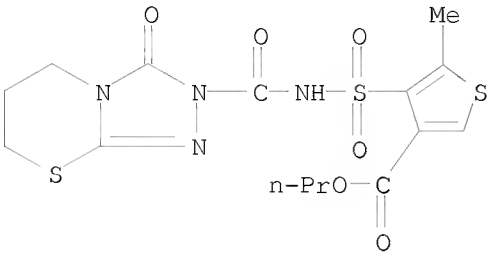


RN 517885-09-5 CAPLUS

CN 3-Thiophenecarboxylic acid, 4-[[[(6,7-dihydro-3-oxo-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-2(3H)-yl)carbonyl]amino]sulfonyl]-5-methyl-, ethyl ester (CA INDEX NAME)



RN 517885-48-2 CAPLUS
CN 3-Thiophenecarboxylic acid, 4-[[[(6,7-dihydro-3-oxo-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-2(3H)-yl)carbonyl]amino]sulfonyl]-5-methyl-, propyl ester (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:598914 CAPLUS
DOCUMENT NUMBER: 130:81472
TITLE: Addition-Cyclization Reactions of Cinnamoyl Isothiocyanate with Nitrogen and Oxygen Nucleophiles
AUTHOR(S): Ahmed, A. F. Sayed; Aouf, N.; Assy, M. G.
CORPORATE SOURCE: Faculty of Science, Chemistry Department, Zagazig University, Zagazig, Egypt
SOURCE: Journal of Chemical Research, Synopses (1998), (9), 508-509, 2056-2061
CODEN: JRPSDC; ISSN: 0308-2342
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
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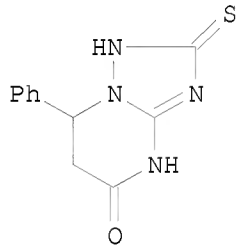

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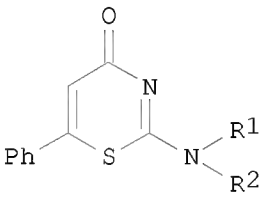

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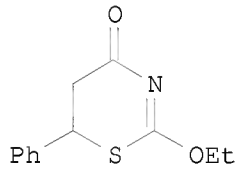

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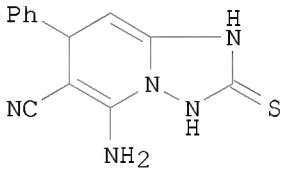

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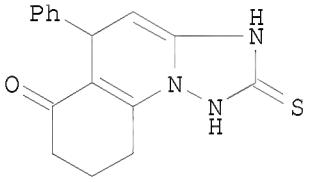

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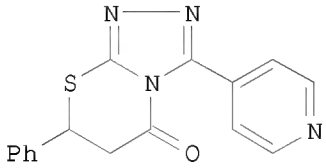
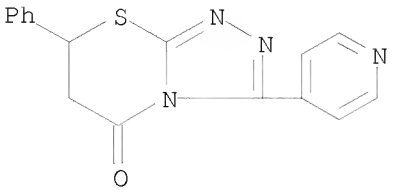


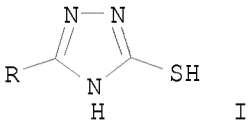
VI

AB Conversions of cinnamoyl isothiocyanate to heterocycles I, II (R1 = R2 = benzyl; R1 = Me, R2 = Ph), III, IV, V, and VI are described.
IT 218438-57-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(addition-cyclization reactions of cinnamoyl isothiocyanate with nitrogen and oxygen nucleophiles)
RN 218438-57-4 CAPLUS
CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazin-5-one, 6,7-dihydro-7-phenyl-3-(4-pyridinyl)- (CA INDEX NAME)

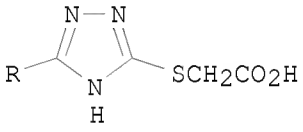


REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1998:18718 CAPLUS
DOCUMENT NUMBER: 128:48174
TITLE: Study on the nucleophilic substitution of 3-aryl-5-mercapto-1,2,4-triazoles
AUTHOR(S): Wang, Zhong-Yi; You, Tian-Pa; Shi, Hai-Jian; Shi, Hao-Xin
CORPORATE SOURCE: Dep. Chem., Univ. Sci. Technol. China, Anhui, 230026, Peop. Rep. China
SOURCE: Youji Huaxue (1997), 17(6), 535-541
CODEN: YCHHDX; ISSN: 0253-2786
PUBLISHER: Kexue Chubanshe
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
GI



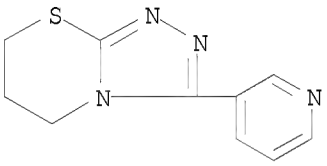
I



II

AB Reaction of title compds. I (R = Ph, 2-MeOC6H4, 2-HOC6H4, 3-O2NC6H4, 4-O2NC6H4, β-pyridyl) with Et bromoacetate, chloroacetic acid, 1,2-dichloroethane, and 1,3-dibromopropane were reported. E.g., reaction of I with chloroacetic acid in EtOH in the presence of NaOH gave triazoles II. II (R = Ph) showed bactericidal and anticancer activities.

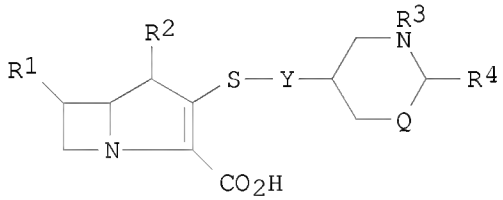
IT 169517-99-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(nucleophilic substitution of 3-aryl-5-mercapto-1,2,4-triazole)
RN 169517-99-1 CAPLUS
CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazine, 6,7-dihydro-3-(3-pyridinyl)- (CA INDEX NAME)



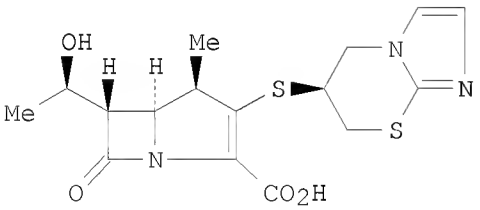
L10 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:623169 CAPLUS
DOCUMENT NUMBER: 127:278102
TITLE: Preparation of carbapenems for use as antibacterial agents
INVENTOR(S): Miwa, Tetsuo; Soejima, Seizo
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 109 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9733888	A1	19970918	WO 1997-JP756	19970311
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, GH, HU, IL, IS, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, YU				
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
JP 10045758	A	19980217	JP 1997-54668	19970310
AU 9722337	A	19971001	AU 1997-22337	19970311
PRIORITY APPLN. INFO.:			JP 1996-52865 A	19960311
			JP 1996-137276 A	19960530
			WO 1997-JP756 W	19970311

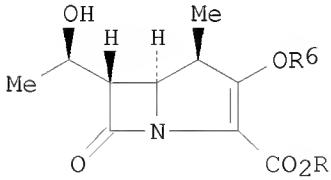
OTHER SOURCE(S): MARPAT 127:278102
GI



I



II



III

AB Carbapenems I [R1 = substituted alkyl; R2 = H, alkyl; Y = bond, alkylene group; Q = O, S; R3R4 = nitrogen containing heterocyclic ring] were prepd and showed excellent antibacterial activities, stability, and absorbability through oral administration. Thus, the sodium salt of carbapenem II was prepared via the coupling ester III [R5 = 4-nitrobenzyl, R6 = P(O)(OPh)2] with 5-benzoylthio-6,7-dihydro-5H-imidazo[2,1-b]thiazine followed by

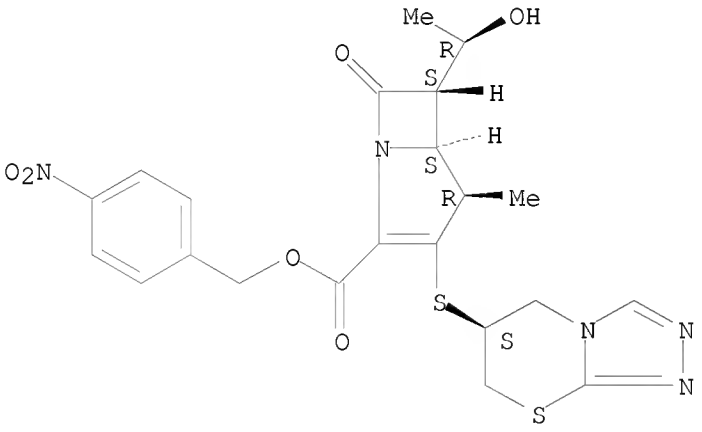
hydrogenation in the presence of Pd. Carbapenem II gave MIC values of 0.05 and 0.025 μg/mL when tested against 106 CFU/mL test suspensions of E. coli NIHJ JC-2 and H. influenzae NN400 bacteria strains, resp.

IT 196602-68-3P 196602-69-4P 196602-70-7P
196602-71-8P 196602-76-3P 196602-77-4P
196602-78-5P 196602-79-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of carbapenems for use as antibacterial agents)

RN 196602-68-3 CAPLUS

CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, (4-nitrophenyl)methyl ester, [4R-[3(S*),4α,5β,6β(R*)]]- (9CI) (CA INDEX NAME)

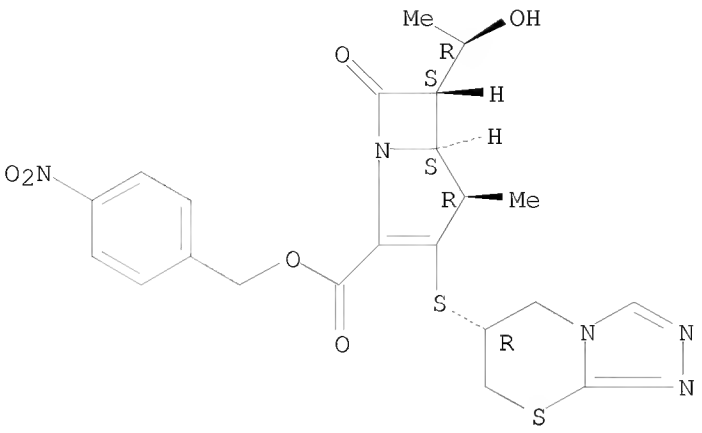
Absolute stereochemistry.



RN 196602-69-4 CAPLUS

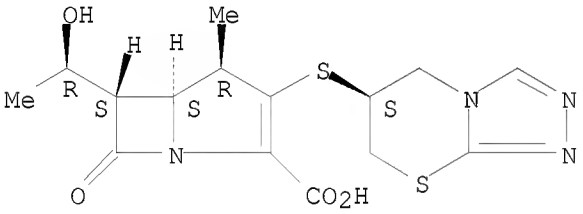
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, (4-nitrophenyl)methyl ester, [4R-[3(R*),4α,5β,6β(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 196602-70-7 CAPLUS
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, monosodium salt, [4R-[3(S*),4α,5β,6β(R*)]]- (9CI) (CA INDEX NAME)

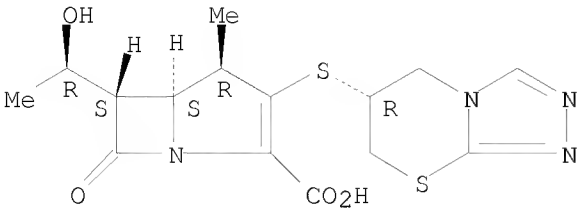
Absolute stereochemistry.



● Na

RN 196602-71-8 CAPLUS
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, monosodium salt, [4R-[3(R*),4α,5β,6β(R*)]]- (9CI) (CA INDEX NAME)

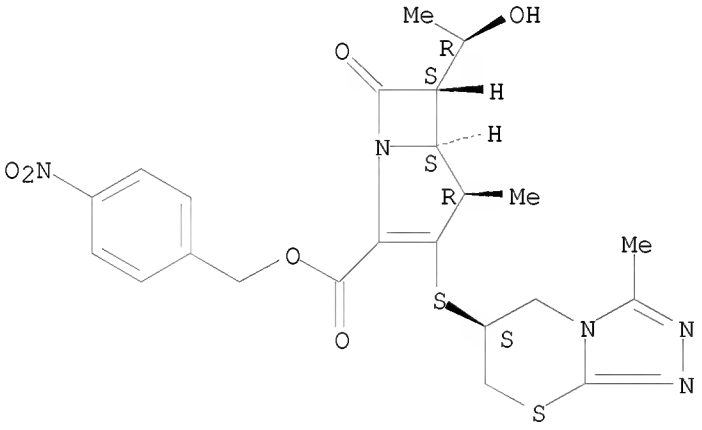
Absolute stereochemistry.



● Na

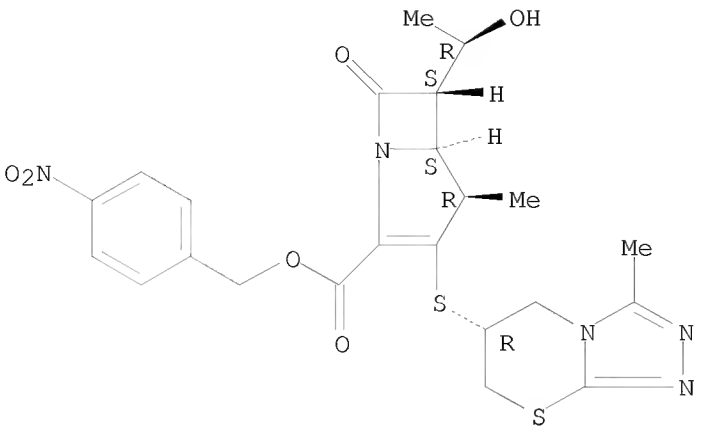
RN 196602-76-3 CAPLUS
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-3-methyl-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, (4-nitrophenyl)methyl ester, [4R-[3(S*),4α,5β,6β(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



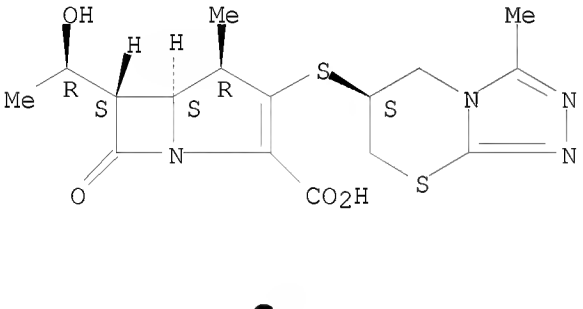
RN 196602-77-4 CAPLUS
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-3-methyl-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, (4-nitrophenyl)methyl ester, [4R-[3(R*),4α,5β,6β(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



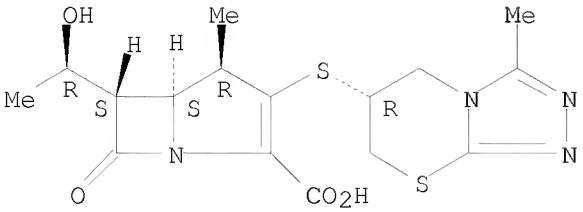
RN 196602-78-5 CAPLUS
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-3-methyl-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, monosodium salt, [4R-[3(S*),4α,5β,6β(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 196602-79-6 CAPLUS
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-3-methyl-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, monosodium salt, [4R-[3(R*),4α,5β,6β(R*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

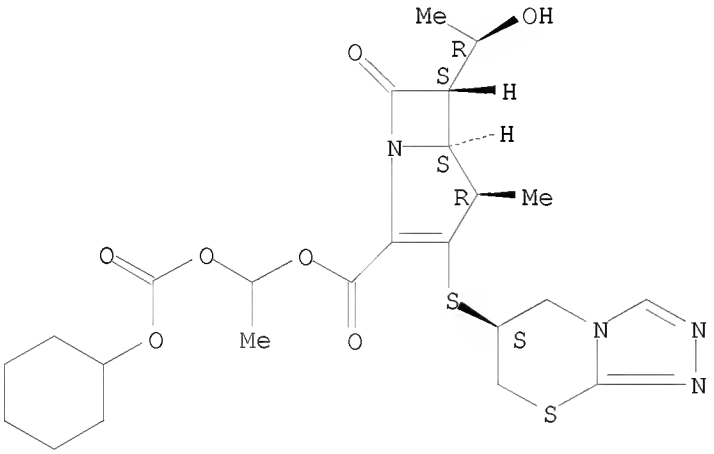


IT 196602-10-5P 196602-11-6P 196602-15-0P
196602-16-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of carbapenems for use as antibacterial agents)

RN 196602-10-5 CAPLUS

CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, 1-[[(cyclohexyloxy)carbonyl]oxy]ethyl ester, [4R-[3(S*),4α,5β,6β(R*)]]-[partial]- (9CI) (CA INDEX NAME)

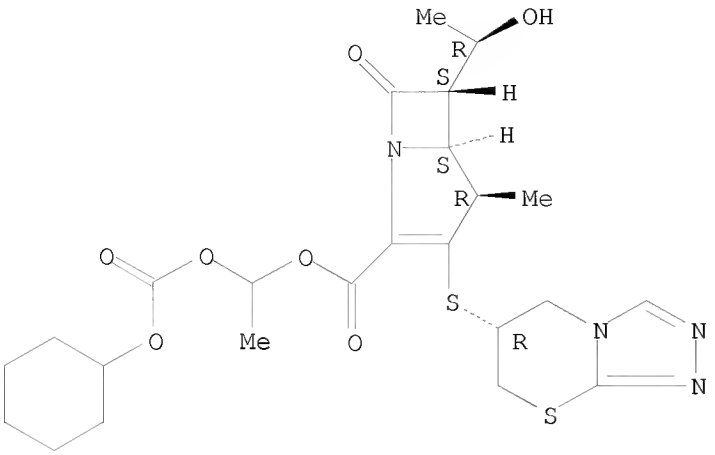
Absolute stereochemistry.



RN 196602-11-6 CAPLUS

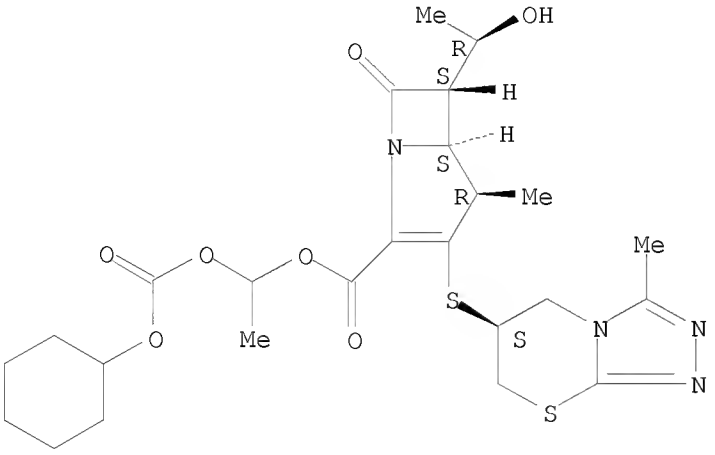
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, 1-[[(cyclohexyloxy)carbonyl]oxy]ethyl ester, [4R-[3(R*),4α,5β,6β(R*)]]-[partial]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



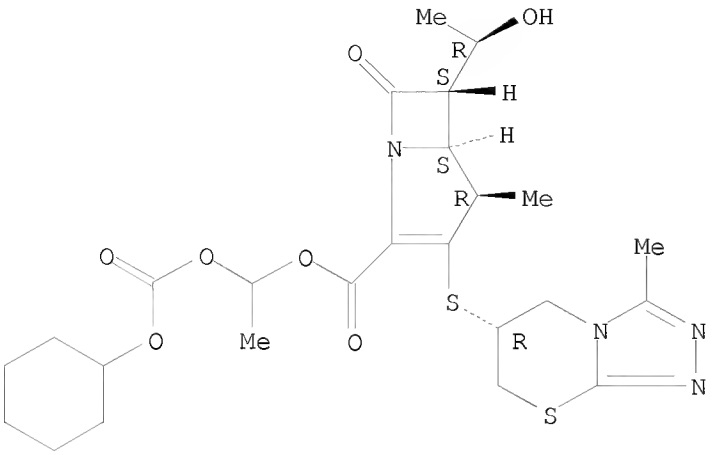
RN 196602-15-0 CAPLUS
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-3-methyl-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, 1-[[(cyclohexyloxy)carbonyl]oxy]ethyl ester, [4R-[3(S*),4α,5β,6β(R*)]]-[partial]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

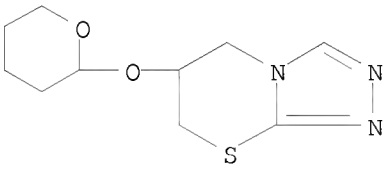


RN 196602-16-1 CAPLUS
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-3-methyl-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, 1-[[(cyclohexyloxy)carbonyl]oxy]ethyl ester, [4R-[3(R*),4α,5β,6β(R*)]]-[partial]- (9CI) (CA INDEX NAME)

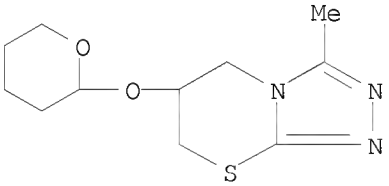
Absolute stereochemistry.



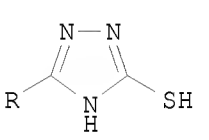
IT 196602-98-9P 196603-11-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of carbapenems for use as antibacterial agents)
RN 196602-98-9 CAPLUS
CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazine, 6,7-dihydro-6-[(tetrahydro-2H-pyran-2-yl)oxy]- (CA INDEX NAME)

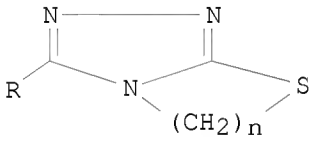


RN 196603-11-9 CAPLUS
CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazine, 6,7-dihydro-3-methyl-6-[(tetrahydro-2H-pyran-2-yl)oxy]- (CA INDEX NAME)

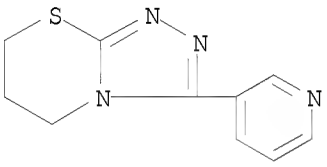


L10 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:685539 CAPLUS
DOCUMENT NUMBER: 123:285879
TITLE: Synthesis of 2-aryl-5,6-dihydrothiazolo[2,3-c]-S-triazoles and 3-aryl-6,7-dihydro-S-triazolo[3,40-b][1,3]thiazines
AUTHOR(S): Wang, Zhongyi; Shi, Haijian; Shi, Haoxin; Zhang, Ziyi
CORPORATE SOURCE: Dep. Chem., Anhui Normal Univ., Wuhu, 241000, Peop. Rep. China
SOURCE: Huaxue Tongbao (1995), (2), 46-8
CODEN: HHTPAU; ISSN: 0441-3776
PUBLISHER: Kexue
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
GI


I


II

AB Reaction of triazolethiols I (R = Ph, substituted Ph, 3-pyridyl) with Cl(CH2)nCl (n = 2, 3) in isopropanol in the presence of KOH-NaHCO3 gave 30.9-89.2% the title compds. II.
IT 169517-99-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of aryldihydrothiazolotriazoles and aryldihydrotriazolothiazines)
RN 169517-99-1 CAPLUS
CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazine, 6,7-dihydro-3-(3-pyridinyl)- (CA INDEX NAME)

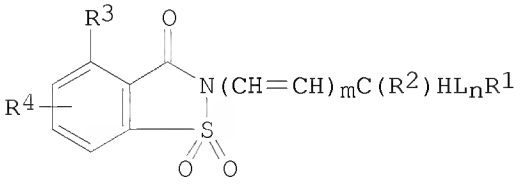


L10 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1994:191707 CAPLUS
DOCUMENT NUMBER: 120:191707
TITLE: 2-Substituted saccharin derivative proteolytic enzyme inhibitors
INVENTOR(S): Hlasta, Dennis John; Desai, Ranjit Chimanlal; Subramanyam, Chakrapani; Lodge, Eric Piatt; Dunlap, Richard Paul; Boaz, Neil Warren; Mura, Albert Joseph; Latimer, Lee Hamilton
PATENT ASSIGNEE(S): Sterling Winthrop Inc., USA
SOURCE: Eur. Pat. Appl., 77 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 7
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 542372	A1	19930519	EP 1992-203469	19921112
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
US 5236917	A	19930817	US 1991-793033	19911115
AU 9225340	A	19930520	AU 1992-25340	19920925
AU 654581	B2	19941110		
CA 2079822	A1	19930516	CA 1992-2079822	19921005
NO 9204401	A	19930518	NO 1992-4401	19921113
NO 303119	B1	19980602		
HU 66873	A2	19950130	HU 1992-3566	19921113
IL 103748	A	19970218	IL 1992-103748	19921113
RU 2101281	C1	19980110	RU 1992-4381	19921113
JP 05194444	A	19930803	JP 1992-305295	19921116
US 5371074	A	19941206	US 1993-67637	19930524
US 5650422	A	19970722	US 1994-270964	19940705
US 5596012	A	19970121	US 1995-449152	19950524
US 5874432	A	19990223	US 1997-803297	19970220

PRIORITY APPLN. INFO.:
US 1991-793033 A 19911115
US 1989-347125 B2 19890504
US 1989-347126 B2 19890504
US 1990-514920 B2 19900426
US 1993-67637 A3 19930524
US 1994-270964 B3 19940705

OTHER SOURCE(S): MARPAT 120:191707
GI



I

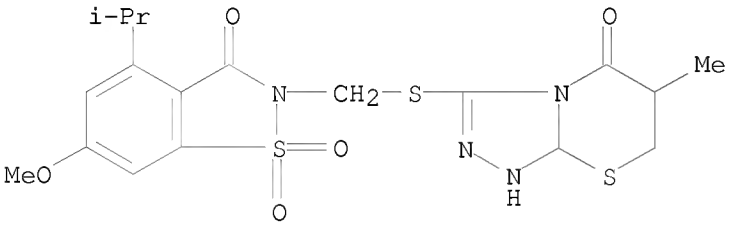
AB The title compds. I [L = O, S, SO, SO2; R1 = (un)substituted Ph,

(un)substituted heterocyclyl, etc.; R2 = H, lower alkoxycarbonyl, Ph, PhS; R3 = H, halogen, (un)substituted alkyl, Ph, lower alkoxy, lower alkoxycarbonyl, CN, etc.; R4 = H or 1-3 substituents selected from halogen, CN, NO2, NH2, etc.; m, n = 0, 1; when m = 0 then R1 can only be heterocyclyl and CHR2 can only be bonded to a ring N of R1; when m = 0, n = 1 and L is O, S, or SO, then R2-R4 = H; when m = 0, n = 1, L is S, R2, R4 = H and R3 = halogen; when m = 0, n = 1, and L is SO or SO2 then R2 is lower alkoxycarbonyl and R3 = R4 = H while R1 ≠ substituted Ph], useful for the treatment of degenerative diseases (no data), are prepared Thus, 2-hydroxymethyl-4-chlorosaccharin was reacted with thionyl chloride, producing 2-chloromethyl-4-chlorosaccharin (II). II demonstrated inhibition constant for human leukocyte elastase (rate of reactivation of enzyme to rate of inactivation of enzyme) of 0.5 nM and 26 nM for α-chymotrypsin.

IT 152177-61-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and proteolytic enzyme inhibitory activity of)

RN 152177-61-2 CAPLUS

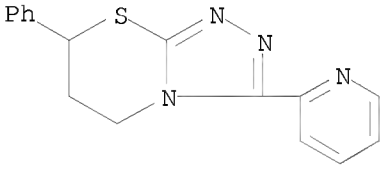
CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazin-5-one, 1,6,7,8a-tetrahydro-3-[[[6-methoxy-4-(1-methylethyl)-1,1-dioxido-3-oxo-1,2-benzisothiazol-2(3H)-yl]methyl]thio]-6-methyl- (CA INDEX NAME)



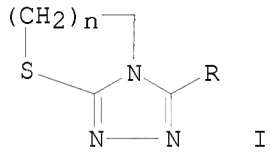
L10 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:81752 CAPLUS
DOCUMENT NUMBER: 114:81752
ORIGINAL REFERENCE NO.: 114:13957a,13960a
TITLE: Cyclization of N1-(cinnamylthiocarbamoyl)amidrazones. Part I
AUTHOR(S): Strzemecka, Leokadia
CORPORATE SOURCE: Inst. Bas. Chem. Sci., Sch. Med., Lublin, 20081, Pol.
SOURCE: Polish Journal of Chemistry (1990), 64(1-6), 157-66
CODEN: PJCHDQ; ISSN: 0137-5083
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:81752

AB The cyclization of R1N:CRNHNHCSNHCH2CH:CHPh (I, R = Ph, R1 = H, Ph; R = 2-pyridyl, R1 = Ph) with HCl has been studied. 1,2,4-Triazole, 1,3,4-thiadiazole, 1,2,4-triazolo[3,4-b]1,3-thiazine and 1,3,4-thiadiazolo[3,2-a]pyrimidine derivs. were obtained in good yields. With dilute HCl I (R = Ph, R1 = H) yielded both triazole and thiadiazole derivs., whereas I (R = Ph, 2-pyridyl, R1 = Ph) yielded only thiadiazoles. The cyclization reaction with concentrated HCl gave the condensed heterocycles.

IT 132065-97-5P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in cyclization of cinnamylthiocarbamoylamidrazone)
RN 132065-97-5 CAPLUS
CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazine, 6,7-dihydro-7-phenyl-3-(2-pyridinyl)- (CA INDEX NAME)

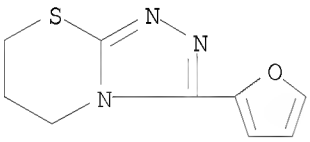


L10 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1980:76416 CAPLUS
DOCUMENT NUMBER: 92:76416
ORIGINAL REFERENCE NO.: 92:12587a,12590a
TITLE: A novel one-step synthesis of 3-substituted-5,6-dihydrothiazolo[2,3-c]-1,2,4-triazoles and -6,7-dihydro-5H-1,2,4-triazolo[3,4-b][1,3]thiazines
AUTHOR(S): Payne, L. G.; Wu, M. T.; Patchett, A. A.
CORPORATE SOURCE: Merck Sharp and Dohme Res. Lab. Div., Merck and Co., Inc., Rahway, NJ, 07065, USA
SOURCE: Heterocycles (1979), 12(9), 1171-4
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 92:76416
GI



I

AB The title compds. I (n = 1, 2; R = 2-furyl, 4-ClC6H4, 3-pyridyl, 4-MeC6H4, Me, Pr, 3-indolylmethyl) were obtained in 35-80% yield by treating RCONHNH2 with ClCH2(CH2)nNCS in the presence of NEt3.
IT 72647-26-8P 72647-34-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 72647-26-8 CAPLUS
CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazine, 3-(2-furanyl)-6,7-dihydro- (CA INDEX NAME)



RN 72647-34-8 CAPLUS
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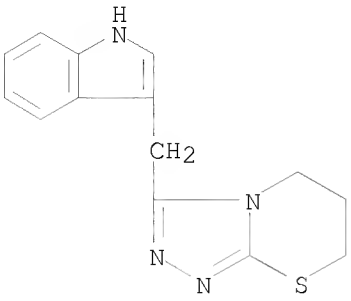
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N
N
S

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E1 THROUGH E60 ASSIGNED

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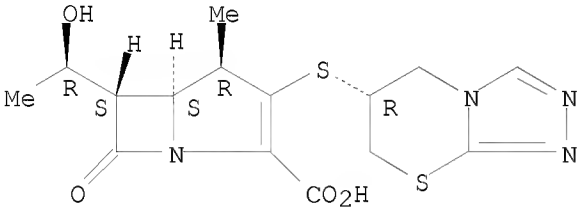
L15 ANSWER 20 OF 25 REGISTRY COPYRIGHT 2008 ACS on STN
RN 777835-35-5 REGISTRY
ED Entered STN: 10 Nov 2004
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[[(6R)-6,7-dihydro-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl]thio]-6-[(1R)-1-hydroxyethyl]-4-methyl-7-oxo-, (4R,5S,6S)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, [4R-[3(R*),4α,5β,6β(R*)]]- (9CI)
FS STEREOSEARCH
MF C15 H18 N4 O4 S2
CI COM
SR CA

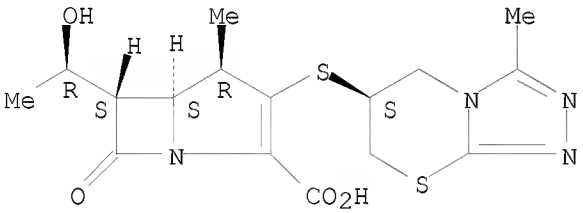
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L15 ANSWER 21 OF 25 REGISTRY COPYRIGHT 2008 ACS on STN
RN 774519-79-8 REGISTRY
ED Entered STN: 04 Nov 2004
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[[(6S)-6,7-dihydro-3-methyl-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl]thio]-6-[(1R)-1-hydroxyethyl]-4-methyl-7-oxo-, (4R,5S,6S)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-3-methyl-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, [4R-[3(S*),4α,5β,6β(R*)]]- (9CI)
FS STEREOSEARCH
MF C16 H20 N4 O4 S2
CI COM
SR CA

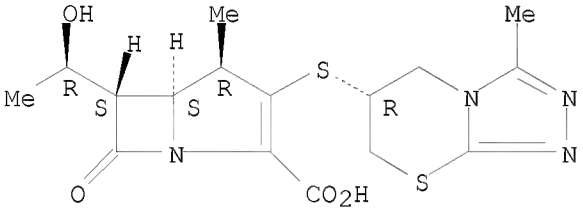
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

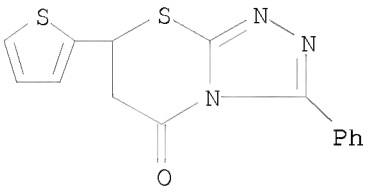
L15 ANSWER 22 OF 25 REGISTRY COPYRIGHT 2008 ACS on STN
RN 764629-48-3 REGISTRY
ED Entered STN: 17 Oct 2004
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[[(6R)-6,7-dihydro-3-methyl-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl]thio]-6-[(1R)-1-hydroxyethyl]-4-methyl-7-oxo-, (4R,5S,6S)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-3-methyl-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, [4R-[3(R*),4α,5β,6β(R*)]]- (9CI)
FS STEREOSEARCH
MF C16 H20 N4 O4 S2
CI COM
SR CA

Absolute stereochemistry.



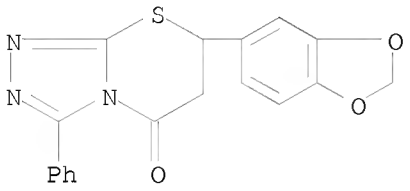
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L15 ANSWER 23 OF 25 REGISTRY COPYRIGHT 2008 ACS on STN
RN 327094-22-4 REGISTRY
ED Entered STN: 14 Mar 2001
CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazin-5-one, 6,7-dihydro-3-phenyl-7-(2-thienyl)- (CA INDEX NAME)
MF C15 H11 N3 O S2
SR Chemical Library
Supplier: Oak Samples Ltd.



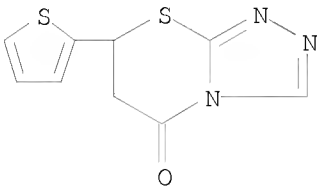
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L15 ANSWER 24 OF 25 REGISTRY COPYRIGHT 2008 ACS on STN
RN 327094-16-6 REGISTRY
ED Entered STN: 14 Mar 2001
CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazin-5-one, 7-(1,3-benzodioxol-5-yl)-6,7-dihydro-3-phenyl- (CA INDEX NAME)
MF C18 H13 N3 O3 S
SR Chemical Library
Supplier: Oak Samples Ltd.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L15 ANSWER 25 OF 25 REGISTRY COPYRIGHT 2008 ACS on STN
RN 325693-79-6 REGISTRY
ED Entered STN: 05 Mar 2001
CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazin-5-one, 6,7-dihydro-7-(2-thienyl)-
(CA INDEX NAME)
MF C9 H7 N3 O S2
SR Chemical Library
Supplier: Oak Samples Ltd.
LC STN Files: CHEMCATS



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L16 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2008 ACS on STN
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ED Entered STN: 14 Mar 2001
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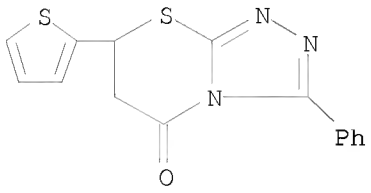
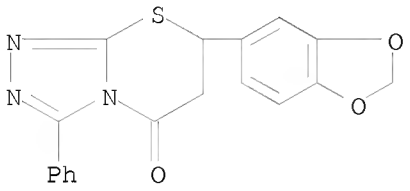
MF C15 H11 N3 O S2
SR Chemical Library
Supplier: Oak Samples Ltd.



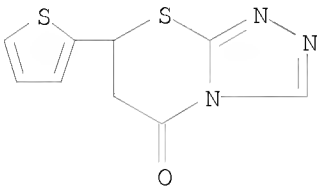
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2008 ACS on STN
RN 327094-16-6 REGISTRY
ED Entered STN: 14 Mar 2001
CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazin-5-one, 7-(1,3-benzodioxol-5-yl)-6,7-dihydro-3-phenyl- (CA INDEX NAME)
MF C18 H13 N3 O3 S
SR Chemical Library
Supplier: Oak Samples Ltd.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L16 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2008 ACS on STN
RN 325693-79-6 REGISTRY
ED Entered STN: 05 Mar 2001
CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazin-5-one, 6,7-dihydro-7-(2-thienyl)-
(CA INDEX NAME)
MF C9 H7 N3 O S2
SR Chemical Library
Supplier: Oak Samples Ltd.
LC STN Files: CHEMCATS



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L3          52 S L1 SSS FUL
L4             STRUCTURE UPLOADED
L5           4 S L4  SUB=L3 FUL
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L7           1 S L5 AND CAPLUS/LC

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L17 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:962262 CAPLUS
DOCUMENT NUMBER: 143:248419
TITLE: Preparation of heterocyclic-fused 1,3-diazenes and analogs as metabotropic glutamate receptor antagonists
INVENTOR(S): Johansson, Martin; Wensbo, David; Minidis, Alexander; Staaf, Karin; Kers, Annika; Edwards, Louise; Isaac, Methvin; Stefanac, Tomislav; Slassi, Abdelmalik; McLeod, Donald
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; NPS Pharmaceuticals, Inc.
SOURCE: PCT Int. Appl., 69 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2005080397	A2	20050901	WO 2005-US5218		20050217
WO 2005080397	A3	20051222			
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CA 2556320	A1	20050901	CA 2005-2556320		20050217
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OTHER SOURCE(S): MARPAT 143:248419
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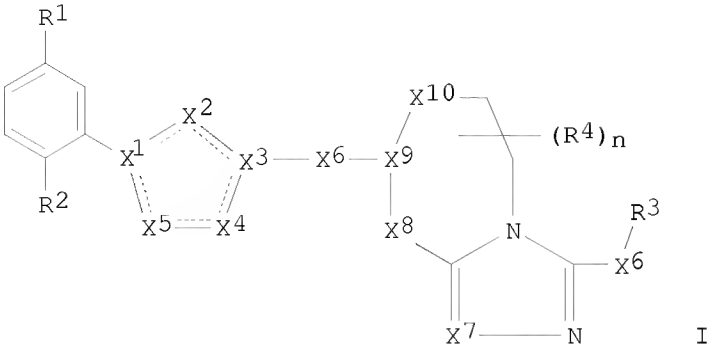


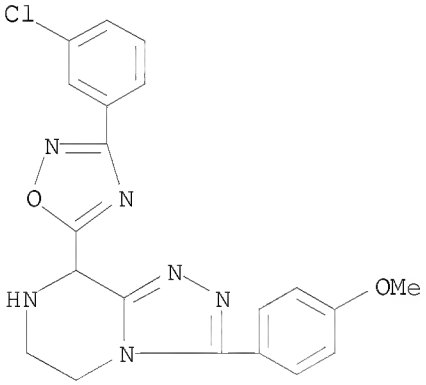
I

AB Title compds. I [X1-5 = C, CR5, N, O, S wherein at least one is not N; X6 = bond, divalent carbon; X7 = CR5, N; X8 = bond, divalent carbon, etc.; X9 = CR5, N; X10 = bond, divalent carbon, etc.; R1 = OH, halo, NO2, etc.; R2 = H, OH, halo, etc.; R3 = 5-6 membered ring; R4 = OH, halo, NO2, etc.; R5 = H, alkyl, cycloalkyl, aryl; n = 0-4 with some provisions] are prepared For instance, 7-[5-(5-Chloro-2-fluorophenyl)-1,2,4-oxadiazol-3-yl]-3-(2-thienyl)-6,7-dihydro-5H-[1,2,4]triazolo[3,4-b][1,3]thiazine is prepared by cyclization of 2-[3-[[[5-(5-chloro-2-fluorophenyl)-1,2,4-oxadiazol-3-yl]methyl]thio]-5-(2-thienyl)-4H-1,2,4-triazol-4-yl]ethyl methanesulfonate (DMF, NaH). Compds. of the invention have IC50 < 10 μM for the mGluR5 receptor. I are useful for the treatment of gastrointestinal disorders.

IT 863307-72-6P, 8-[3-(3-Chlorophenyl)-[1,2,4]oxadiazol-5-yl]-3-(4-methoxyphenyl)-5,6,7,8-tetrahydro-[1,2,4]triazolo[4,3-a]pyrazine
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of heterocyclic-fused 1,3-diazenes and analogs as metabotropic glutamate receptor antagonists)

RN 863307-72-6 CAPLUS

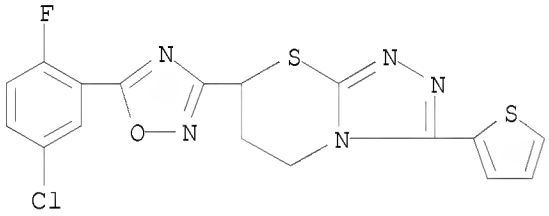
CN 1,2,4-Triazolo[4,3-a]pyrazine, 8-[3-(3-chlorophenyl)-1,2,4-oxadiazol-5-yl]-5,6,7,8-tetrahydro-3-(4-methoxyphenyl)- (CA INDEX NAME)



IT 863307-58-8P, 7-[5-(5-Chloro-2-fluorophenyl)-1,2,4-oxadiazol-3-yl]-3-(2-thienyl)-6,7-dihydro-5H-[1,2,4]triazolo[3,4-b][1,3]thiazine

863307-59-9P, 9-[[5-(3-Chlorophenyl)-1,2,4-oxadiazol-3-yl]methyl]-3-(pyridin-4-yl)-6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a][1,3]diazepine 863307-60-2P, 9-[[5-(3-Chlorophenyl)isoxazol-3-yl]methyl]-3-(3,5-difluorophenyl)-6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a][1,3]diazepine 863307-61-3P, 9-[[5-(3-Chlorophenyl)isoxazol-3-yl]methyl]-3-(4-methoxyphenyl)-6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a][1,3]diazepine 863307-63-5P, 9-[[5-(3-Chlorophenyl)isoxazol-3-yl]methyl]-3-(pyridin-4-yl)-6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a][1,3]diazepine 863307-65-7P, 9-[[5-(5-Chloro-2-fluorophenyl)-1,2,4-oxadiazol-3-yl]methyl]-3-(pyridin-4-yl)-6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a][1,3]diazepine 863307-66-8P, 9-[[5-(3-Chlorophenyl)-1,2,4-oxadiazol-3-yl]methyl]-3-(3,5-difluorophenyl)-6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a][1,3]diazepine 863307-68-0P, 9-[[5-(3-Chlorophenyl)-1,2,4-oxadiazol-3-yl]methyl]-3-(4-methoxyphenyl)-6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a][1,3]diazepine 863307-69-1P, 9-[1-[5-(3-Chlorophenyl)-1,2,4-oxadiazol-3-yl]ethyl]-3-(pyridin-4-yl)-6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a][1,3]diazepine 863307-70-4P, 7-[[5-(3-Chlorophenyl)-1,2,4-oxadiazol-3-yl]methyl]-3-(pyridin-4-yl)-6,7-dihydro-5H-pyrrolo[2,1-c][1,2,4]triazole 863307-71-5P, 9-[[5-(3-Chlorophenyl)-1,2,4-oxadiazol-3-yl]methyl]-3-(trifluoromethyl)-6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a][1,3]diazepine 863307-73-7P, 8-[3-(3-Chlorophenyl)-[1,2,4]oxadiazol-5-yl]-3-(4-methoxyphenyl)-7-methyl-5,6,7,8-tetrahydro-[1,2,4]triazolo[4,3-a]pyrazine
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclic-fused 1,3-diazenes and analogs as metabotropic glutamate receptor antagonists)

RN 863307-58-8 CAPLUS
CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazine, 7-[5-(5-chloro-2-fluorophenyl)-1,2,4-oxadiazol-3-yl]-6,7-dihydro-3-(2-thienyl)- (CA INDEX NAME)



RN 863307-59-9 CAPLUS
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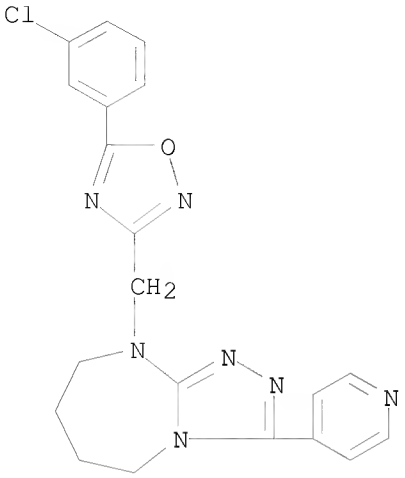

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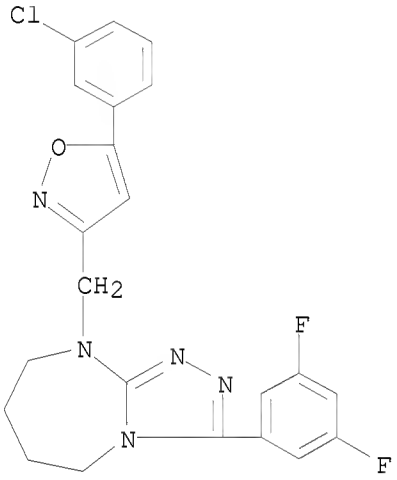
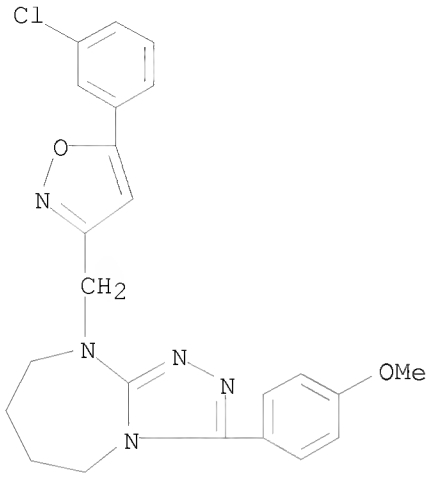
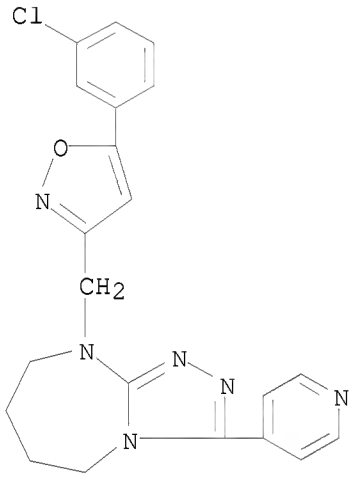


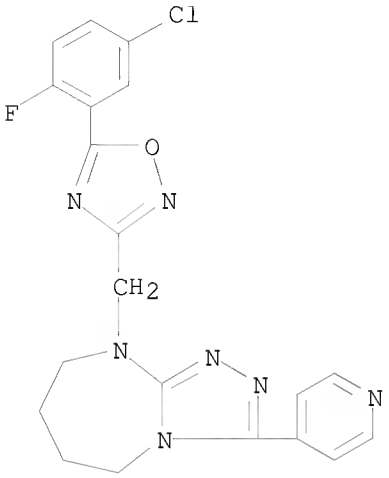
RN 863307-61-3 CAPLUS
CN 5H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 9-[[5-(3-chlorophenyl)-3-isoxazolyl]methyl]-6,7,8,9-tetrahydro-3-(4-methoxyphenyl)- (CA INDEX NAME)



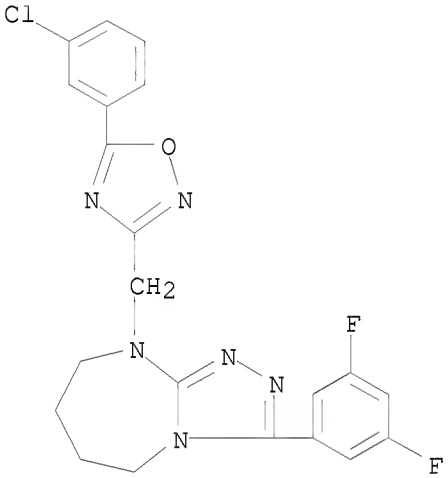
RN 863307-63-5 CAPLUS
CN 5H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 9-[[5-(3-chlorophenyl)-3-isoxazolyl]methyl]-6,7,8,9-tetrahydro-3-(4-pyridinyl)- (CA INDEX NAME)



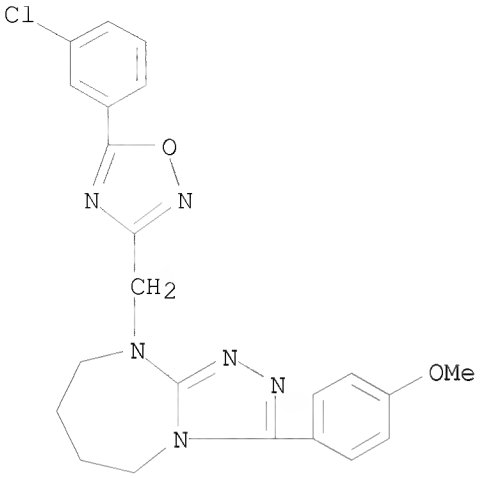
RN 863307-65-7 CAPLUS
CN 5H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 9-[[5-(5-chloro-2-fluorophenyl)-1,2,4-oxadiazol-3-yl]methyl]-6,7,8,9-tetrahydro-3-(4-pyridinyl)- (CA INDEX NAME)



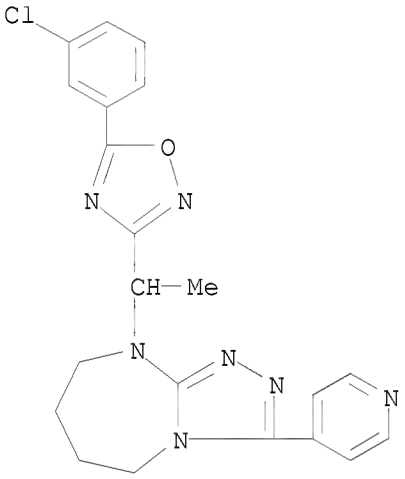
RN 863307-66-8 CAPLUS
CN 5H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 9-[[5-(3-chlorophenyl)-1,2,4-oxadiazol-3-yl]methyl]-3-(3,5-difluorophenyl)-6,7,8,9-tetrahydro- (CA INDEX NAME)



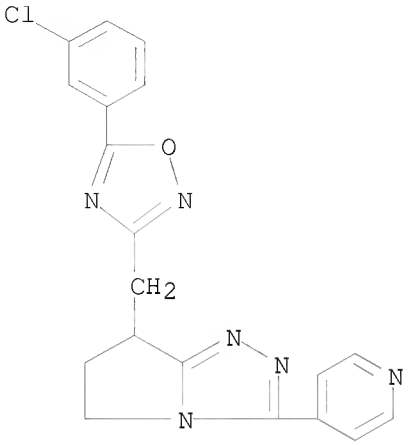
RN 863307-68-0 CAPLUS
CN 5H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 9-[[5-(3-chlorophenyl)-1,2,4-oxadiazol-3-yl]methyl]-6,7,8,9-tetrahydro-3-(4-methoxyphenyl)- (CA INDEX NAME)



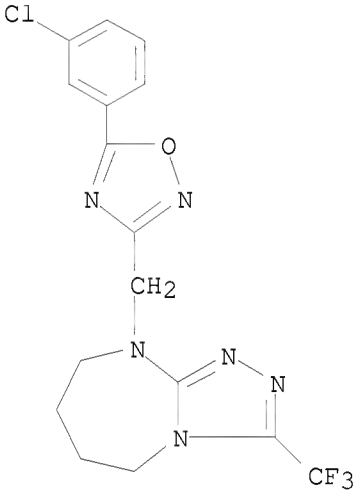
RN 863307-69-1 CAPLUS
CN 5H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 9-[1-[5-(3-chlorophenyl)-1,2,4-oxadiazol-3-yl]ethyl]-6,7,8,9-tetrahydro-3-(4-pyridinyl)- (CA INDEX NAME)



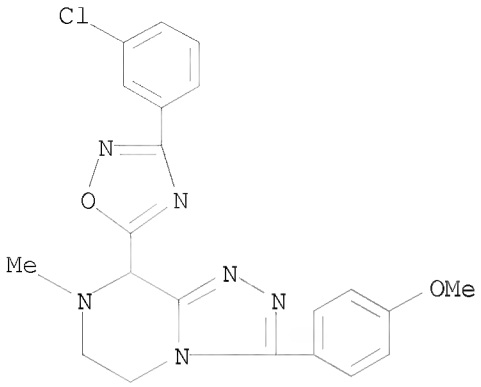
RN 863307-70-4 CAPLUS
CN 5H-Pyrrolo[2,1-c]-1,2,4-triazole, 7-[[5-(3-chlorophenyl)-1,2,4-oxadiazol-3-yl]methyl]-6,7-dihydro-3-(4-pyridinyl)- (CA INDEX NAME)



RN 863307-71-5 CAPLUS
CN 5H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 9-[[5-(3-chlorophenyl)-1,2,4-oxadiazol-3-yl]methyl]-6,7,8,9-tetrahydro-3-(trifluoromethyl)- (CA INDEX NAME)

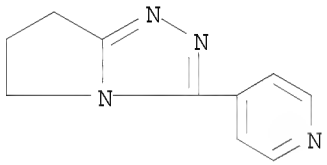


RN 863307-73-7 CAPLUS
CN 1,2,4-Triazolo[4,3-a]pyrazine, 8-[3-(3-chlorophenyl)-1,2,4-oxadiazol-5-yl]-5,6,7,8-tetrahydro-3-(4-methoxyphenyl)-7-methyl- (CA INDEX NAME)

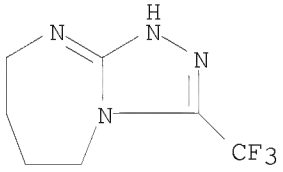


IT 114722-58-6P, 3-(Pyridin-4-yl)-6,7-dihydro-5H-pyrrolo[2,1-c][1,2,4]triazole 148461-26-1P, 3-(Trifluoromethyl)-6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a][1,3]diazepine 775260-07-6P, 3-(Pyridin-4-yl)-6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a][1,3]diazepine 863307-49-7P, 3-(3,5-Difluorophenyl)-6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a][1,3]diazepine 863307-50-0P, 3-(4-Methoxyphenyl)-6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a][1,3]diazepine 863307-57-7P, 8-[3-(3-Chlorophenyl)-[1,2,4]oxadiazol-5-yl]-3-(4-methoxyphenyl)-5,6-dihydro-8H-[1,2,4]triazolo[4,3-a]pyrazine-7-carboxylic acid tert-butyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heterocyclic-fused 1,3-diazenes and analogs as metabotropic glutamate receptor antagonists)

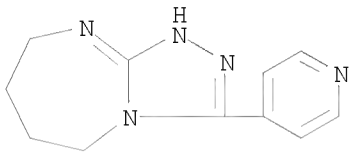
RN 114722-58-6 CAPLUS
CN 5H-Pyrrolo[2,1-c]-s-triazole, 6,7-dihydro-3-(4-pyridinyl)- (6CI, 9CI) (CA INDEX NAME)



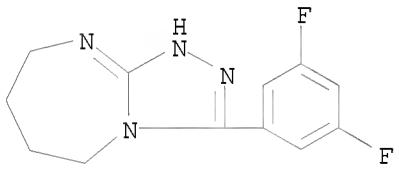
RN 148461-26-1 CAPLUS
CN 1H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 5,6,7,8-tetrahydro-3-(trifluoromethyl)- (CA INDEX NAME)



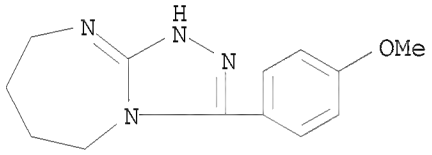
RN 775260-07-6 CAPLUS
CN 1H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 5,6,7,8-tetrahydro-3-(4-pyridinyl)- (CA INDEX NAME)



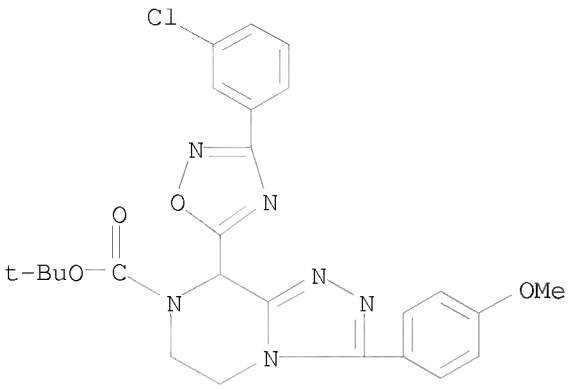
RN 863307-49-7 CAPLUS
CN 1H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 3-(3,5-difluorophenyl)-5,6,7,8-tetrahydro- (CA INDEX NAME)



RN 863307-50-0 CAPLUS
CN 1H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 5,6,7,8-tetrahydro-3-(4-methoxyphenyl)- (CA INDEX NAME)



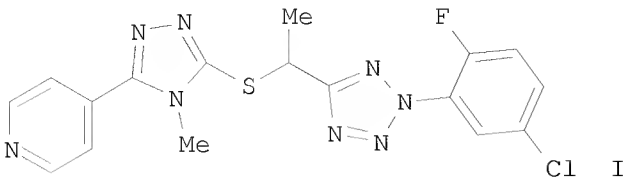
RN 863307-57-7 CAPLUS
CN 1,2,4-Triazolo[4,3-a]pyrazine-7(8H)-carboxylic acid, 8-[3-(3-chlorophenyl)-1,2,4-oxadiazol-5-yl]-5,6-dihydro-3-(4-methoxyphenyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)


Cl
N
O
N
O
t-BuO
C
N
N
N
N
OMe

L17 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:962228 CAPLUS
DOCUMENT NUMBER: 143:266932
TITLE: Preparation of tetrazole compounds and their use as metabotropic glutamate receptor antagonists
INVENTOR(S): Johansson, Martin; Minidis, Alexander; Staaf, Karin; Wensbo, David; McLeod, Donald; Edwards, Louise; Isaac, Methvin; O'Brien, Anne; Slassi, Abdelmalik; Xin, Tao
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; NPS Pharmaceuticals, Inc.
SOURCE: PCT Int. Appl., 118 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2005080356	A1	20050901	WO 2005-US5217		20050217
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
AU 2005214379	A1	20050901	AU 2005-214379		20050217
CA 2556263	A1	20050901	CA 2005-2556263		20050217
EP 1716125	A1	20061102	EP 2005-713793		20050217
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, BA, HR, IS, YU					
CN 1918137	A	20070221	CN 2005-80004370		20050217
BR 2005007498	A	20070710	BR 2005-7498		20050217
JP 2007523182	T	20070816	JP 2006-554236		20050217
US 20060004021	A1	20060105	US 2005-60463		20050218
NO 2006003470	A	20061117	NO 2006-3470		20060728
IN 2006DN04470	A	20070810	IN 2006-DN4470		20060802
KR 2007027504	A	20070309	KR 2006-715943		20060807
MX 2006PA09019	A	20070308	MX 2006-PA9019		20060808
US 20070197549	A1	20070823	US 2007-588756		20070309
PRIORITY APPLN. INFO.:			US 2004-545291P	P	20040218
			WO 2005-US5217	W	20050217

OTHER SOURCE(S): MARPAT 143:266932
GI

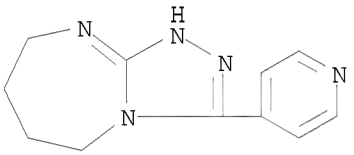


I

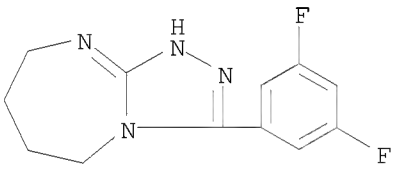
AB The present invention relates to new tetrazole compds., or salts, solvates or solvated salts thereof, processes for their preparation and new intermediates used in the preparation thereof, pharmaceutical compns. containing said compds., and to the use of said compds. in therapy. E.g., I was prepared from 1-[2-(5-chloro-4-phenyl)-2H-tetrazol-5-yl]ethyl methanesulfonate, K2CO3, and 4-methyl-5-pyridin-4-yl-2,4-dihydro-[1,2,4]triazole-3-thione in MeCN. IC50 values for glutamate receptor assays were given for I and Et 4-[1-[2-(3-chlorophenyl)-2H-tetrazol-5-yl]ethyl]piperazine-1-carboxylate.

IT 775260-07-6P 863307-49-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of tetrazole compds. and their use as metabotropic glutamate receptor antagonists)

RN 775260-07-6 CAPLUS
CN 1H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 5,6,7,8-tetrahydro-3-(4-pyridinyl)- (CA INDEX NAME)

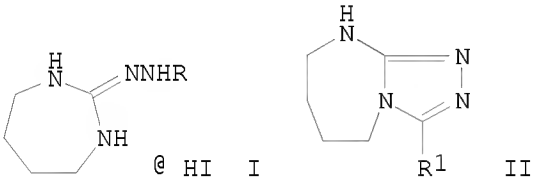


RN 863307-49-7 CAPLUS
CN 1H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 3-(3,5-difluorophenyl)-5,6,7,8-tetrahydro- (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1993:449358 CAPLUS
DOCUMENT NUMBER: 119:49358
ORIGINAL REFERENCE NO.: 119:8957a,8960a
TITLE: Synthesis of 1,2,4-triazolo[4,3-a](1,3)diazepines. Reactions of hexahydro-1H-1,3-diazepin-2-one hydrazone hydroiodide with acyl reagents. Part 7: 1,2,4-triazolo[4,3-a]diazacycloalkanes
AUTHOR(S): Krezel, Izabella
CORPORATE SOURCE: Dep. Pharm. Chem. Drug Anal., Med. Acad., Lodz, Pol.
SOURCE: Pharmazie (1993), 48(3), 189-92
CODEN: PHARAT; ISSN: 0031-7144
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

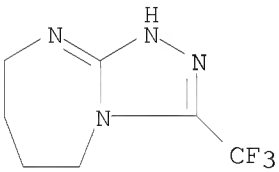


AB Reactions of hexahydro-1H-1,3-diazepin-2-one hydrazone hydroidide I (R = H) with different acyl reagents are described. Reaction of I with R1COCl (R1 = Ph, 2-thienyl, CF3, PhCH2, etc.) affords, in acetonitrile, I (R = COR1), while in pyridine, the reaction products are derivs. of 1,2,4-triazolo[4,3-a](1,3)diazepines II. From the reaction of I (R = H) with trifluoroacetic anhydride, a mixture of I (R = COCF3) and II (R1 = CF3) was obtained. With acetic anhydride and I (R = H), acetyltriazolodiazepine III was obtained, while the reaction with trifluoroacetic acid affords, depending on reaction conditions, I (R = COCF3) or II (R1 = CF3).

IT 148461-26-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 148461-26-1 CAPLUS

CN 1H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 5,6,7,8-tetrahydro-3-(trifluoromethyl)- (CA INDEX NAME)



L17 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1961:38138 CAPLUS
DOCUMENT NUMBER: 55:38138
ORIGINAL REFERENCE NO.: 55:7450h-i,7451a-e
TITLE: 1,2,4-Triazole derivatives
PATENT ASSIGNEE(S): Farbenfabriken Bayer Akt.-Ges.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 825514		19591216	GB 1956-36166	19561126

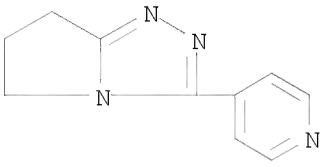
GI For diagram(s), see printed CA Issue.

AB Triazole derivs., CH2.(CH2)n.N.C:N.N:CR (I), useful as analeptics and as central nervous system and respiratory system stimulants, were prepared from CH2.(CH2)n.C(OMe):N (II) and appropriate hydrazides. II (n = 4) (45 g.) added dropwise to 48.3 g. p-O2NC6H4CONHNH2 in 500 g. hot alc., the mixture refluxed 1 hr., and filtered gave p-O2NC6H4CONHNH-C:N.(CH2)4.CH2 (III), m. 188-97°. III (50 g.) heated with 200 g. AcOH and diluted with H2O gave 30% I (n = 4, R = p-O2NC6H4), m. 184-5° [MeOCH2CH2OAc (IV)]. Hydrogenation of this compound gave I (n = 4, R = p-H2NC6H4), m. 210-12°. Compds. prepared similarly were: CH:CH.N:CH.CH:CCONHNHC:N.(CH2)4.CH2, m. 208-10°; I (n = 4, R = 4-pyridyl) hydrochloride, m. 248-55° (sinters at 245°); CH:N.CH:CH.CH:CCONHNHC:N.(CH2)4.CH2, m. 107-8° (from IV); and I (n = 4, R = 3-pyridyl), m. 81-2° (from IV). Prepared from II (n = 4) and the appropriate hydrazide without isolation of the intermediate were the following I (n = 4, R and m.p. given): H, about 65° (b16 239-41°; hydrochloride, m. 228-30°); NCCH2, 112-13° (hydrochloride, m. 253-5°); MeOCH2, - (hydrochloride, m. 156-8°); Ph, 132-4°; p-ClC6H4, 171° (from IV); 2,4-Cl2C6H3, 130-2° (EtOAc); p-MeOC6H1, 157-9°; o-HOC6H4, 260-5° (HCONMe2); α-furyl, 151-3° (EtOAc); H2NCO, 189-90° (hydrochloride decomposed at 245°); o-MeOC6H4, 160-1° (alc.); and 3-hydroxy-2-naphthyl, 306-8°. II (n = 4) and H2NNHCSNHNHCSOEt gave I (n = 4, R = NHNHCSOMe), m. 198-200°. II (n = 4) and (H2NNHCOCH2CH2)2 gave butylenebis I derivative (n = 4), m. 139-41°. Similarly the following I (n = 2) were prepared from II (n = 2) and the appropriate hydrazide (R and m.p. given): H (V), 65° (b0.6 200-2°; hydrochloride, m. 195-7°); H2NCO. 182-3°; 4-pyridyl (VI), -; butylenebis compound, 247-9° (H2O). OHCNHNH-C:N.(CH2)2.CH2 and CH:CH.N:CH.CH:CHCONHNH-C:N.(CH2)2.CH2, intermediates in the preparation of V and VI, m. 138–40° and 127-8°, resp. II (n = 3) and (H2NNHCOCH2CH2)2 gave 80–90% butylenebis I derivs. (n = 3), m. 185-6° (from IV). II (n = 3) and CH:CH.N:CH.CH:-CCONHNH2 gave 90% I (n = 3, R = 4-pyridyl), m. 165-6°. Similarly II (n = 6) and the appropriate hydrazide gave I (n = 6, R = H), I (n = 6, R = H2NCO), m. 176-8°, and I (n = 6, R = 4-pyridyl), m. 117-19° (C6H6) [hydrochloride, m. 115-17° (H2O)].

IT 114722-58-6P, 5H-Pyrrolo[2,1-c]-s-triazole, 6,7-dihydro-3-(4-pyridyl)-
RL: PREP (Preparation)
(preparation of)

RN 114722-58-6 CAPLUS

CN 5H-Pyrrolo[2,1-c]-s-triazole, 6,7-dihydro-3-(4-pyridinyl)- (6CI, 9CI) (CA INDEX NAME)



L17 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1960:50526 CAPLUS
DOCUMENT NUMBER: 54:50526
ORIGINAL REFERENCE NO.: 54:9960e-i,9961a
TITLE: Cycloalkanotriazoles and intermediates
INVENTOR(S): Petersen, Siegfried; Tietze, Ernst; Wirth, Wolfgang
PATENT ASSIGNEE(S): Schenley Industries, Inc.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2913454		19591117	US 1956-623828	19561123

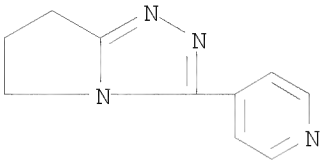
GI For diagram(s), see printed CA Issue.

AB The title compds. are prepared by treating a cyclic lactim ether of 5-10 C atoms with an acylhydrazine at 0-150°. They are useful as analeptics, stimulants, for the central nervous and respiratory systems, and intermediates in various syntheses. Thus, over 0.5 hr. caprolactim O-methyl ether 140 is added at 20°, without cooling, to monoformylhydrazine 60, in MeOH 400 parts (the temperature rises to 55°). After the mixture reaches 25°, it is refluxed on a H2O-bath 15 hrs., MeOH and H2O are distilled in vacuo at 100°, and the residue is distilled in vacuo from a metal bath to yield 4,5-pentamethylene-1,2,4-triazole 129 parts (94%), b16 239-41°, m. approx. 65° (hygroscopic colorless crystals); hydrochloride, m. 228-30° (decomposition). The following compds. are also prepared: 3-methoxymethyl-4,5-pentamethylene-1,2,4-triazole, b15 225-8°, viscous colorless oil; hydrochloride m. 156-8°; 3-phenyl-4,5-pentamethylene-1,2,4-triazole, brown crystals m. 132-4°; 3-(4-nitrophenyl)-4,5-pentamethylene-1,2,4-triazole, pale yellow crystals, m. 184-5°, prepared by ring closure of the intermediate m. 188-97°; 3-(o-hydroxyphenyl)-4,5-pentamethylene-1,2,4-triazole m. 260-5°; 3-(4-pyridyl)-4,5-pentamethylene-1,2,4-triazole, deliquescent crystals whose hydrochloride sinters at 245° and m. 248-55° and which is prepared from the intermediate 2-(2-benzoylhydrazino)-1-aza-1-cycloheptene, m. 208-10°; 3-(2-furyl)-4,5-pentamethylene-1,2,4-triazole, m. 151-3°; 3-carbamoyl-4,5-pentamethylene-1,2,4-triazole, m. 189-90°; hydrochloride decomposing at 245°; 3-(2-ethoxythiocarbonylhydrazino)-4,5-pentamethylene-1,2,4-triazole, needles, m. 198-200°; 3-cyanomethyl-4,5-pentamethylene-1,2,4-triazole, m. 112-13°; hydrochloride m. 253-5° (decomposition); 1,4-bis(4,5-tetramethylene-1,2,4-triazol-3-yl)butane, m. 139-41°; 4,5-tetramethylene-3-methyl-1,2,4-triazole, b14 224°, m. 85-6° (monohydrate m. 54-5°); 4,5-heptamethylene-1,2,4-triazole, viscous oil; 2-(2-methoxyhydrazino)-3,4,5,6,7-pentahydroazepine; 2-thiosemicarbazido-3,4,5,6,7-pentahydroazepine; and 2-(2-benzenesulfonylhydrazino)-3,4,5,6,7-pentahydroazepine.

IT 114722-58-6P, 5H-Pyrrolo[2,1-c]-s-triazole, 6,7-dihydro-3-(4-pyridyl)-
RL: PREP (Preparation)
(preparation of)

RN 114722-58-6 CAPLUS

CN 5H-Pyrrolo[2,1-c]-s-triazole, 6,7-dihydro-3-(4-pyridinyl)- (6CI, 9CI) (CA INDEX NAME)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L17 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1958:50690 CAPLUS
DOCUMENT NUMBER: 52:50690
ORIGINAL REFERENCE NO.: 52:9158a-i,9159a-c
TITLE: Reactions of cyclic lactim ethers with acylhydrazine derivatives
AUTHOR(S): Petersen, Siegfried; Tietze, Ernst
CORPORATE SOURCE: Farbenfabrik Bayer, Leverkusen, Germany
SOURCE: Chemische Berichte (1957), 90, 909-21
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 52:50690
GI For diagram(s), see printed CA Issue.
AB The previously reported (Schlack, C.A. 39, 14201) H2C.(CH2)4.N:COMe (I) (30 g.) added to 20 g. H2NNHC:N.N:N.NH in 250 cc. EtOH at 50°, boiled 30 min. on an H2O bath, and filtered hot yielded 31 g. H2C.(CH2)4.N:CR (II) (R = NHNHC:N.N:N.NH), m. 225° (decomposition) (H2O), with MeOH splitting off. I (30 g.) in 300 cc. EtOH similarly treated at 60° with 39.4 g. o-C6H4.SO2.N:CNHNH2 yielded 26 g. II (R = o-C6H4.SO2.N:CNHNH), m. 197-8° (HCONMe2-H2O), whereas 30 g. I with 32.8 g. H2NN.CH:N.N:CH in 250 cc. EtOH needed 10 hrs. heating in an autoclave at 140°/10 atmospheric to yield 35 g. II (R = HNN.CH:N.N:CH), m. 242°. With R'CONHNH2 (III) I gave II (R = R'CONHNH) (IV) as above, or by splitting off H2O from the enol form of IV H2C.(CH2)4.N.C:N.N:CR' (V). Thus, 45 g. I added to 48.3 g. III (R ' = 4-O2NC6H4) in 500 cc. MeOH at 60° and boiled 1 hr. yielded 65 g. IV (R' = 4-O2NC6H4) (VI), m. 188°; and similarly I with III (R' = 4-pyridyl) gave IV (R' = 4-pyridyl) (VII), m. 210°. However, 140 g. I added dropwise to 60 g. III (R' = H) in 400 cc. MeOH at 20° during 30 min. while the temperature rose to 55°, the mixture refluxed 15 hrs., and distilled in vacuo yielded 129 g. V (R' = H), b16 239-41°, m. 65°; HCl salt, m. 228-30°. Likewise, I with III (R' = NCCH2, Ph, or 2-furyl) gave V (R' = NCCH2, Ph, or 2-furyl), m. 111° (HCl salt, m. 244°), 133°, and 152°, resp. That V were formed through IV was proved by obtaining both IV and V from a single compound in many cases, IV at lower temperature and shorter reaction time. Thus, 50.8 g. I added dropwise to 29.6 g. III (R' = Me) in 200 cc. MeOH at 0-5° with stirring (1 hr.) and kept 15 hrs. at 0° yielded 45 g. IV (R' = Me), m. 176-7° (decomposition) (HCl salt, m. 181°); 74 g. III (R' = Me) in 500 cc. MeOH and 140 g. I quickly mixed without cooling, refluxed 15 hrs., and distilled in vacuo yielded 133 g. V (R' = Me), b16 235-7°, m. 108° (HCl salt, m. 213-15°), formed also by refluxing IV (R' = Me) 15 hrs. in MeOH. Likewise, 50 g. VI boiled 5 min. in 200 cc. AcOH, cooled to 80°, and 200 cc. H2O added yielded 40 g. V (R' = O2NC6H4), m. 184°. This ease of ring closure was shown by the catalytic reduction (Raney Ni) of 50 g. VI whereby 45 g. V (R' = H2NC6H4) was formed [not IV (R' = H2NC6H4)], m. 211°, also formed by the catalytic reduction of V (R' = O2NC6H4). VII was also converted to the corresponding V (HCl salt, m. 248-55°) by boiling 5 min. in AcOH. Other similar compds. were prepared (compound, R', and m.p. given): IV, Et, 169°; IV, 3-pyridyl, 108°; V, Et, 41° (b0.05 164°); V, H2NCO, 191°; V, MeOCH2, b15 226° (HCl salt, m. 157°); V, p-ClC6H4, 171°; V, 2,4-Cl2C6H3, 131°; V, o-HOC6H4, 260-5°; V, o-MeOC6H4, 161°; V, p-MeOC6H4, 158°; V, 2,3-HOC10H6, 309°; V,

3-pyridyl, 81°. Noteworthy were the reactions of I with (CH2)4(CONHNH2)2, H2NNHCO2Et, H2NNHCSNH2, H2NNHSO2Ph, and H2NNHCSNHNHCSOEt under conditions similar to the preceding to give, resp.: bis V compound [R' = (CH2)4], m. 140°; IV (R' = CO2Et), m. 122°, and then by longer heating and splitting off of EtOH instead of H2O, V (R' = HO), m. 179°; IV (R' = CSNH2), m. 240-50° (decomposition); IV (R' = SO2Ph), m. 190-1°; and V (R' = NHNHCSOEt), m. 198-200°. Finally it was found that H2C.(CH2)x.N:COMe (VIII) (x = 2, 3, or 6) reacted as I did. According to Benson and Cairns (C.A. 42, 6749e) 252 g. Me2SO4 added dropwise with stirring to 170 g. H2C.(CH2)x.N:COH (IX) (x = 2) in 100 cc. C6H6 at 60-70°, the mixture refluxed 8 hrs., cooled to 5°, 150 g. K2CO3 quickly added, then 100 cc. H2O added dropwise with cooling (1 hr.) while CO2 evolved and the temperature rose to 20°, and the C6H6 layer distilled in vacuo yielded 95 g. VIII (x = 2), b. 118-21°, rearranged by heating 1-2 hrs. at 120-5° to H2C.(CH2)x.NMe.CO (X) (x = 2), b. 198-200°, b12 82-3°. Similar treatment converted IX (x = 6) at 75% VIII (x = 6), b14 89°, b0.1 61-2°, rearranged to X (x = 6), b14 140°. R' and m.p. (in parentheses) for IV prepared from VIII (x = 2) were: H (139°), Me (194°), EtO (151°), 4-pyridyl (227°). For V prepared from VIII (x = 2): H (HCl salt, m 196°), Me (HCl salt, m. 200°), HO (179°), H2NCO (181°), 4-pyridyl (186°), (CH2)4 (bis V compound) (247°). For IV prepared from VIII (x = 6): EtO (132°). For V prepared from VIII (x = 3): Me (86°) (b14 224°), HO (131°), 4-pyridyl (166°), (CH2)4 (bis V compound) (184°). For V prepared from VIII (x = 6): H (b0.1 167°), Me (40°) (b0.6 172°) (HCl salt, m. 168°), HO (112°), H2NCO (177°), MeOCH2 (b0.2 188°), Ph (113°), 3-pyridyl (104°), 4-pyridyl (119°) (HCl salt, m. 216°), (CH2)4 (bis V compound) (112°).

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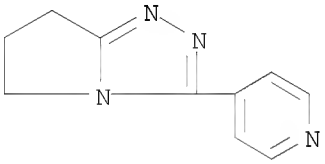
RL: PREP (Preparation)
(preparation of)

RN 114722-58-6 CAPLUS

CN 5H-Pyrrolo[2,1-c]-s-triazole, 6,7-dihydro-3-(4-pyridinyl)- (6CI, 9CI) (CA INDEX NAME)



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